Neutron Diffraction Study of 4-nitroaniline at 100K

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The planarity of the amino group in nitroanilines is still a matter of controversy. It has been assumed in several experimental and theoretical studies of 4-nitroaniline (pNA) [1]. Single crystal X-ray diffraction and experimental electron density analysis of pNA have been previously reported [2,3]. However, no accurate experimental coordinates and atomic displacement parameters (adps) for the hydrogen atoms are available yet. As shown by Bürgi et al. [4], accurate adps for hydrogen atoms are essential for obtaining reliable results on physical properties. With this in mind, we have carried out a single crystal neutron diffraction study of pNA at 100K. It shows a relationship between the planarity of the amino moiety and the degree of intramolecular charge transfer, as well as a hydrogen bond scheme different from that observed in other primary anilines [1].

[1] Goeta A. E., et al., *Chem Mater.*, 2000, **12**, 3342, *and references therein*. [2] Tonogaki M., et al., *Acta Cryst. B*, 1993, **49**, 1031. [3] Coppens P., Volkov A., *Acta Cryst. A*, 2004, **60**, 357. [4] Bürgi H. B., et al., C*hem.Eur.J.,* 2002, **8**, 3512.

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